Materials Science Forum 1997 vol.255-257, pages 145-149

Positron states and annihilation characteristics at semiconductor surfaces

Fazleev N., Fry J., Weiss A.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Experimental PAES spectra from the (100) and (111) surfaces of Ge display several strong Auger peaks in the measured energy range corresponding to M4,5N1N2,3 M2,3M4,5M4,5 M2,3M4,5V , and M1M2,3N1,2,3 Auger transitions. Theoretical analysis of PAES data is performed within the modified superimposed-atom method. Positron surface states are computed for both surfaces of Ge. It is found that the positron surface-state wave function is localized mainly on the vacuum side of the topmost layer of Ge atoms. The computed positron binding energies Eb at the (100) and (111) surfaces of Ge are 3.14 and 2.96 eV. In addition, calculations of positron work functions with respect to the vacuum for bulk Ge(100) and Ge(111) yielded 2.77 and 2.85 eV, respectively demonstrating the stability of positron surface states on these surfaces. The positron surface-state lifetime and probabilities for a positron trapped in a surface state to annihilate with relevant core-level electrons are computed for both surfaces. A comparison with PAES data reveals that the modified superimposedatom method gives correct order of magnitude results for the Auger transitions considered.

Keywords

Annihilation, Auger, Position, Semiconductor, Structure, Surface